

US EPA ARCHIVE DOCUMENT

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Date Out of EAB: MAR 26 1985

To: Henry Jacoby
Product Manager 21
Registration Division (TS-767)

From: Samuel Creeger, Chief
Review Section #1
Exposure Assessment Branch
Hazard Evaluation Division (TS-769)

- ① hydrolysis
- ② o/w partition
- ③ soil metabolism
- ④ leaching
- ⑤ adsorption/desorption

Attached, please find the EAB review of...

Reg./File # : 707-EUP-RNL and -RNU

Chemical Name: RH 3866

Type Product : Fungicide

Product Name : RH 3866 40W

Company Name : Rohm and Haas

Purpose : EUP: New chemical : Use on apples, wheat and grapes.

Action Code(s): 710

EAB #(s) : 5242-43

Date Received: 1/7/85

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Deferrals to:

- ☐ Ecological Effects Branch
- ☐ Residue Chemistry Branch
- ☐ Toxicology Branch

1.0 CHEMICAL: RH-3866
αbutyl-α[4-chlorophenyl]-1-H-1,2,4-triazole-1-propanenitrile)

2.0 TEST MATERIAL: Various

3.0 STUDY/ACTION TYPE: EUP use on Apples, Wheat and Grapes

4.0 STUDY IDENTIFICATION:

4.1 Ackerman, I.B. June, 1984. Laboratory leaching study with RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-09. Acc. No. 072909.

4.2 Ackerman, I.B. July, 1984. Laboratory soil metabolism of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-14. Acc. No. 072907.

4.3 Allen, S.S. May, 1984. A hydrolysis study of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-04. Acc. No. 072909.

4.4 Allen, S.S. May, 1984. Adsorptive and desorptive properties of RH-3866 on soils. Rohm and Haas, Philadelphia, PA. Report No. 310-85-05. Acc. No. 072909.

4.5 Allen, S.S. and D.R. Streelman. July, 1983. The octanol/water partition coefficient of RH-3866. Technical Report No. 210-83-18. Rohm and Haas, Philadelphia, PA. Acc. No. 072907.

5.0 REVIEWED BY:

Typed Name : Emil Regelman
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Signature: 

Date: 3/21/85

6.0 APPROVED BY:

Typed Name : Samuel Creeger
Title : Chief
Organization: Review Section #1
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Signature: 

Date: MAR 26 1985

7.0 CONCLUSIONS:

EAB cannot concur with the proposed EUP at this time, since data requirements to support the proposed EUP have not been satisfied.

EAB is in complete concurrence with the following summary, taken in toto from the Dynamac evaluation of the submitted data.

Hydrolysis studies: One study (Allen, 1984, Acc. No. 072909) was submitted and reviewed. This study is scientifically valid. However, in order to satisfy Guidelines Requirements the temperatures at which the test solutions were maintained must be reported.

Aerobic soil metabolism: One study (Ackerman, 1984, Acc. No. 072907) was submitted and reviewed. This study may provide useful data for EUP requirements, however, the incubation temperature must be reported. In addition, for full registration, data from a longer sampling period may be required (Guidelines Requirements are for up to 12 months posttreatment).

Anaerobic soil metabolism: One study (Ackerman, 1984, Acc. No. 072907) was submitted, reviewed and found to be scientifically valid. However, the temperature at which samples were incubated must be reported.

Leaching and adsorption/desorption studies: Two studies (Allen, 1984, Acc. No. 072909 and Ackerman, 1984, Acc. No. 072909) were submitted and reviewed. [By EAB: We consider this requirement as not satisfied in the absence of a good aged leaching study.]

Confined accumulation studies on rotational crops: No data were submitted; all data are required.

Laboratory studies of a accumulation in fish: No bioaccumulation studies were submitted; all data are required.

8.0 RECOMMENDATIONS:

The registrant should review the Dynamac evaluation of their submitted data, and respond to the deficiencies noted in §7.0, above.

9.0 BACKGROUND:

A. Introduction

Rohm and Haas has submitted data to support the proposed EUP use of RH 3866 Fungicide on Apples, Wheat and Grapes. These studies were forwarded to an EPA contractor (DYNAMAC Corp.) for review. EAB concurs with that review, a copy of which is appended.

B. Directions for Use

The proposed EUP label should be submitted for EAB review.

10.0 DISCUSSION OF INDIVIDUAL TESTS OR STUDIES:

A. Study Identification

See §4.0. above

B. Materials and Methods (Protocols)

C. Reported Results

D. Study Author's Conclusions/Quality Assurance Measures

See DYNAMAC review (appended) for a complete discussion of each of the submitted studies.

E. Reviewer's Discussion and Interpretation of Study Results

EAB is in complete concurrence with the following summary, taken in toto from the Dynamac evaluation of the submitted data.

RH-3866 appears stable to hydrolysis at pHs 5, 7, or 9. However, the temperature at which the test solutions were maintained was not reported.

Tentative results (incubation temperature not reported) indicate that RH-3866 is metabolized under aerobic conditions in a silt loam soil to 1,2,4-triazole, CO₂ and a non-extractable form. Initial half-lives were 61 and 71 days respectively for triazole- and phenyl-labeled RH-3866 (calculated from data for up to 62 days of incubation). However, degradation was slower with increased aging; after 240 days up to 37% of recovered ¹⁴C was still present as parent. Tentative results (incubation temperature not reported) indicated that RH-3866 was not appreciably metabolized within 62 days of anaerobic incubation in a silt loam soil.

A batch study indicated that parent RH-3866 was of intermediate mobility in a range of soil types. Aged RH-3866 residues were not extensively leached in a silt loam soil column study.

[By EAB: However, this aged leaching study contains an excessive number of deficiencies which render it invalid.]

Estimates of the octanol/water partition coefficient for RH-3866 ranged from 693 to 957.

11.0 COMPLETION OF ONE-LINER:

No additional data have been added to the one-line data summary.

12.0 CBI APPENDIX:

A copy of the DYNAMAC review is appended to this review. It contains data which the registrant considers to be confidential, and should be handled as such.

RH - 3866

Final Report

**Task 1: Review and Evaluation of
Individual Studies**

**Task 2: Environmental Fate and
Exposure Assessment**

Contract No. 68-01-6679

MARCH 19, 1985

Submitted to:
Environmental Protection Agency
Arlington, VA 22202

Submitted by:
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INTRODUCTION

This document contains scientific evaluations of studies of the environmental fate of RH-3866 submitted under Accession Numbers 072907, 072908, and 072909 (Accession Number 072909 contained appendices to studies only). Experimental program and product use information was submitted under Accession Number 072894.

Diagrams of chemical structures included in the appendix to this report have been redrawn. Tables have been retyped and in many instances reformatted. Data not directly reported by the registrant (i.e., data calculated by the reviewer) are indicated as such either in tables or in the text.

STUDY 1

Ackermann, I.B. July, 1984. Laboratory soil metabolism of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-14. Acc. No. 072907. Ref. Vol. 13, Sec. 21.

Procedure

This study was conducted using field moist (18.4%), sieved (3.45 mm) Lawrenceville silt loam soil (13% sand, 61% silt, 26% clay, 1.2% organic matter, pH 5.3, cation exchange capacity 5.3 meq/100 g, bulk density 1.49 g/cm³, field moisture capacity 27.4%).

Aerobic soil metabolism: Soil samples in quartz jars were treated in triplicate at ~1 ppm with an acetone solution of either uniformly phenyl ring-labeled [¹⁴C]RH-3866, 3,5-triazole-labeled [¹⁴C]RH-3866 or uniformly ring-labeled [¹⁴C]2,4-D [(2,4-dichlorophenoxy)acetic acid]. Characteristics of the test compounds are reported in Table 1. One soil sample treated with acetone only was used as a control. After mixing, subsamples of the treated soils were transferred to aerated flasks with side arms containing sodium hydroxide (15 ml, 0.5 M) to trap evolved CO₂. At intervals up to 367 days posttreatment, 10-g soil samples were removed. Samples from replicate flasks were combined and stored frozen until analysis. Aliquots from the sodium hydroxide traps were removed at the same intervals.

Anaerobic soil metabolism: After 30 days of aerobic incubation, subsamples of Lawrenceville soil treated as described above were submerged in N₂-purged water. Flasks were evacuated and flushed three times with N₂, then sealed. Samples were taken after 15, 32 and 62 days by removing 20 ml of the soil slurry. After each sampling, the flasks were purged (N₂) and re-sealed.

Sterile samples: Four aliquots of Lawrenceville soil were autoclaved for three hours (120°C, 17 psi). Each was then treated with one of the test chemicals or with acetone only as described above (Aerobic soil metabolism). Treated soils were sampled after 6, 14 and 30 days.

Methodology

Radioactivity in the sodium hydroxide traps was quantified by LSC. A subsample of the trap solution was then treated with 2N BaCl₂ to precipitate adsorbed ¹⁴CO₂. The amount of unreacted NaOH was then quantified by titration with HCl to a phenolphthalein end point. Titration values were used to calculate the amount of ¹⁴CO₂ evolved per unit weight of soil.

Anaerobic soil samples were filtered, air-dried, and stored frozen. Subsamples of the filtrate were radioassayed, the remainder was passed through a preconditioned (methanol, then water) reverse-phase Sep-pak cartridge. The Sep-pak was then sequentially eluted with water and methanol. After a subsample was counted the methanol solution was evaporated (N₂). Residues were stored (-20°C) until TLC analysis.

Soil samples were extracted twice by shaking with acetonitrile:acetic acid (70:30). Combined filtered extracts were counted (LSC), diluted with water, and partitioned three times with methylene chloride. Subsamples of the combined methylene chloride phases and of the aqueous phase were radioassayed (LSC). The methylene chloride phase was taken to dryness (rotary evaporator); residues in acetone were again taken to dryness (N_2). The aqueous phase was concentrated under vacuum then taken to dryness (N_2). Residues were stored ($-20^\circ C$) until TLC analysis.

Aerobically aged (150- and 181-day) samples were extracted sequentially with 0.5 M NaOH then 1.0 M NaOH by mixing for 7 and 15 hours respectively. The soil was washed three times with distilled water then three times with 1.0 M NaOH. Subsamples of the centrifuged 0.5 M NaOH extract and the combined 1 M NaOH extracts and washes were assayed for ^{14}C activity (LSC). The NaOH solutions were then each acidified to pH 1 (6 N HCl); precipitated humic acids, separated by centrifugation, were radioassayed (combustion). The fulvic fraction was partitioned three times with ethyl acetate. All fractions were counted (LSC). The combined ethyl acetate phases were evaporated (rotary evaporator). Residues, in methanol, were taken to dryness (N_2) then stored at $-20^\circ C$ for TLC analysis.

Extracted soils were air-dried then stored frozen until analyzed. They were then combusted to quantify (LSC) unextracted ^{14}C -activity.

Soil and water extracts were cochromatographed with reference standards (see Appendix) on silica gel plates containing a fluorescent dye. One of three chloroform:methanol:acetic acid mobile phases [90:10:0.5 (A), 85:15:0.5 (B) or 75:25:1 (C)] were used. Unlabeled standards were located on the plates by visualization under UV light. Radioactive spots were located by autoradiography and quantified by zonal scraping followed by LSC.

Results

Aerobic soil metabolism: Reported total ^{14}C recoveries (based on day zero data) ranged from 81% to 112%. The residue distribution for RH-3866 is summarized in Table 2.

The proportion of activity recovered as extractable parent RH-3866 was similar for the two labels throughout the experimental period. However, the two labeled moieties of degraded parent molecules were metabolized differently. Up to 28% of the ^{14}C from the chlorophenyl moiety was recovered as $^{14}CO_2$; whereas a maximum of 3% was reported for the triazole label. Very little ^{14}C activity was reported in the aqueous soil extract from the phenyl-labeled treatment throughout the experiment. However, there was a steady increase in activity (identified as 1,2,4-triazole) in this fraction with time in the triazole-labeled treatment, up to 15% of recovered activity on day 240. Most of the organosoluble activity from both labels was present as parent; an unidentified polar metabolite comprised <15% of the activity in this fraction.

The extractability of ^{14}C residues into water or organic solvents decreased with increased incubation time. Alkaline extraction of the 150 and 181 day

soil samples removed ~85% of the activity, most of which was recovered in the fulvic acid fraction. Organosoluble residues in this fraction were shown to be present as parent and an unidentified polar metabolite; aqueous soluble residues were not identified.

Approximately 60% of applied radioactivity was respired as $^{14}\text{CO}_2$ from the 2,4-D-treated soils within one year. The metabolism of 2,4-D was not further described.

Anaerobic soil metabolism: Reported total ^{14}C recoveries (based on day zero data) ranged from 97% to 115%.

Throughout the incubation, >90% of recovered activity from both labels was associated with the soil. The reported residue distribution is summarized in Table 3. ^{14}C was largely recovered as unbound parent. The residue distribution was similar for both labels and did not change markedly with increased incubation time.

No results were reported for 2,4-D treated samples.

Sterile samples: After 30 days, ~99% of the triazole label and ~93% of the chlorophenyl label were extracted from soil as parent (reviewer calculated, based on reported application levels). Less than 4% and 3% (for the triazole and chlorophenyl labels, respectively) of the applied activity was recovered from extracted soils on combustion.

Table 1. Characteristics of the test compounds.

Test compound	Specific activity DPM/ μg	Purity (%)	Amount applied to soil (μg)
3,5-triazole- labeled [^{14}C]RH-3866	24,380	99	190
Uniformly phenyl- labeled [^{14}C]RH-3866	22,616	97	255
Uniformly ring- labeled [^{14}C]2,4-D	47,310	98	203

Table 2. Distribution of ^{14}C in triazole- and chlorophenyl-labeled [^{14}C]RH-3866 treated, aerobically incubated silt loam soil.^a

Label position	Incubation time (days)	RH-5076 ^b	RH-3866 ^c	Unidentified		CO ₂	Unextracted
				Polar unknown ^{cd}	Other unknowns ^{ce}		
Triazole	0	ND ^f	98	NR ^g	2	ND	ND
	3	ND	96	NR	2	ND	2
	7	ND	93	1	2	ND	4
	14	ND	87	5	2	ND	6
	21	2	78	8	2	ND	9
	30	4	71	9	2	ND	14
	51	10	63	5	1	1	20
	62	13	54	4	5	1	23
	90	16	41	4	5	1	31
	120	17	42	NR	3	2	38 ⁱ
	150	18	41	NR	NR	3	36 ⁱ
	150 ^h	16	41	4	5	NR	7
	180	18	40	NR	2	2	38 ⁱ
	180 ^h	16	51	3	9	NR	5
	240	15	34	1	3	3	44
Chlorophenyl	0	NR	94	NR	3	0	3
	3	NR	94	1	2	0	3
	7	NR	91	2	2	0	5
	14	NR	85	6	2	1	6
	21	NR	82	5	1	2	10
	30	NR	72	9	2	4	13
	51	1	64	6	1	10	21
	62	1	54	7	2	14	22
	90	1	50	3	3	18	25
	120	1	43	3	2	22	28
	150	2	47	3	1	21	26 ⁱ
	150 ^h	NR	5	4	12.5	NR	5
	180	2	43	NR	NR	25	27 ⁱ
	180 ^h	NR	5	6	15.0	NR	4
	240	1	37	2	3	28	29

^a Expressed as a percent of ^{14}C recovered.

^b Aqueous soluble.

^c Organosoluble.

^d Activity recovered as single polar unknown.

^e Includes 'origin' and other unidentified material.

^f ND, not detected.

^g NR, not reported.

^h Activity recovered in the fulvic acid fraction following alkali extraction.

ⁱ Unextracted prior to alkali extraction.

Table 3. Distribution of ^{14}C in triazole and chlorophenyl- labeled [^{14}C]RH-3866 treated anaerobically incubated silt loam soil.

Label position	Incubation time (days) ^a	Soil			Water	
		RH-3866 ^b	Polar ^b metabolite	Unextracted ^c	RH-3866 ^b	Polar ^b metabolite
Triazole	15	73	2.5	13	3.0	0.2
	32	80	2.0	15	3.0	0.3
	62	78	NR ^d	18	3.0	1.5
Phenyl	15	80	2.0	10	5.0	3.0
	32	77	2.0	15	4.0	3.0
	62	79	2.0	12	5.0	3.0

^a Number of days incubated anaerobically (samples previously incubated aerobically for 30 days).

^b Calculated: % Distribution soil/water x % ^{14}C residues extracted x % component (from TLC).

^c Determined by combustion, expressed as a percentage of total ^{14}C recovered.

^d NR, not reported.

Conclusions

Aerobic soil metabolism: Both triazole- and phenyl-labeled [^{14}C]RH-3866 were metabolized in aerobically incubated Lawrenceville silt loam soil; initial half-lives of 61 days ($r^2 = 0.988$) and 71 days ($r^2 = 0.997$) respectively, were calculated from the data for the first eight samplings (up to 62 days of incubation). However, the data show that degradation rates slowed with increased aging and after 240 days incubation, 34% and 37% of recovered ^{14}C was still present as extractable parent. Analyses of the 367-day samples were not reported. Results from sterile samples indicate that degradation was microbial. Results indicate that RH-3866 is metabolized to 1,2,4-triazole, CO_2 (from mineralization of the phenyl ring), and a non-extractable form. However, intermediates were not identified.

These conclusions are tentative because the incubation temperature was not reported.

Anaerobic soil metabolism: RH-3866 did not degrade appreciably during 62 days anaerobic incubation, at an unspecified temperature, in Lawrenceville silt loam soil. The ratio of parent compound, polar metabolite, and unextractable residue remained constant in the soil and water phases through 62 days.

Incubation temperatures were not reported.

This report was difficult to evaluate because the data were poorly presented. Significant data such as overall ^{14}C recoveries were presented in the extensive appendices only, and were not tabulated nor discussed in the text of the report.

STUDY 2

Allen, S.S. May, 1984. A hydrolysis study of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-04. Acc. No. 072909. Ref. Vol. 15, Sec. 20.

Procedure

Sterile, aqueous buffer solutions (pH 5, 7, and 9) were fortified at 10 ppm with triazole-labeled [^{14}C]RH-3866 (specific activity 10.98 mCi/g, 99% pure. Inventory Lot No 417.0101) in sterile amber bottles. Aliquots of the resultant solutions were stored in capped centrifuge tubes in the dark at ambient temperature. Tubes were sampled after 0, 1, 2, 4, 7, 15, 21, and 28 days.

Methodology

Samples were extracted twice with toluene. The aqueous phase was radioassayed (LSC); combined toluene extracts were evaporated to dryness (40°C, N_2). Residues, in methanol were analyzed by TLC; triplicate aliquots of the methanol solutions were counted (LSC).

TLC analyses were conducted either on reverse-phase plates eluted with methanol:water (85:15), or on silica gel plates eluted with ethyl acetate:isopropanol:water (85:13:2) or chloroform:methanol (90:10). Radioactive areas were located by autoradiography. Quantification was by zonal scraping followed by LSC.

Results

At all pHs, >99% of ^{14}C recovered after 28 days partitioned into toluene. TLC analysis indicated that >99% of this activity was present as unchanged parent.

Conclusions

The reported data suggest that RH-3866 is stable to hydrolysis at pHs 5, 7, or 9 for 28 days.

The temperature at which the solutions were maintained was not reported.

Actual recoveries of RH-3866 commonly exceeded the stated fortification level by at least 10%. The registrant did not discuss this, nor its implications for experimental error.

STUDY 3

Ackermann, I.B. June, 1984. Laboratory leaching study with RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-09. Acc. No. 072909. Ref Vol. 15, Sec. 22.

Procedure

Aliquots of sieved (3.4 mm), field moist (18.4%) Lawrenceville silt loam soil (characteristics reported in Study 1) were treated at ~1 ppm with either 3,5-triazole-labeled [^{14}C]RH-3866, phenyl-labeled [^{14}C]RH-3866 or phenyl-labeled [^{14}C]2,4-D[(2,4-dichlorophenoxy)acetic acid]. Characteristics of the test compounds are reported in Study 1 (Table 1). The treated soils were mixed thoroughly, transferred to biometer flasks and aerobically aged at room temperature for 30 days in CO_2 -free air.

Glass columns (32.5 cm x 7.5 cm wide) were prepared by joining glass rings together. The columns were filled with untreated, sieved, soil and wetted from the bottom up. Columns were drained overnight and additional soil was added, as necessary, to adjust the height of soil in each column to 28 cm. Ninety-five grams of ^{14}C -aged soil was then added to the top of each column. Seven columns were set up, duplicates for each test compound and a single control.

Each day, five days per week, for a total of 46 days, 55 mls of water (equivalent to 1.3 cm or 0.5 inches rainfall) were added dropwise to each column over a 1 to 2 hr period. Leachate volume was measured daily. Water remaining on the top of two soil columns at the end of the experimental period was removed by pipette, for volume measurement and analysis. Columns were divided into component sections: 0 to 5 cm, 5 to 10 cm, 10 to 15 cm, 15 to 22.5 cm and 22.5 to 30 cm. Sections were stored at room temperature in polyethylene bags for two weeks, then weighed and mixed thoroughly.

Methodology

Column eluate, collected every second day, was radioassayed (LSC). Water remaining on the top of two columns was also subjected to LSC.

After moisture content determination soil samples were combusted to determine total ^{14}C content. Evolved $^{14}\text{CO}_2$ was quantified by LSC. Combustion efficiency was determined using soil spiked with a known quantity of ^{14}C sodium benzoate.

Aged soils (pre-leaching) and selected segments of leached soils (0 to 5 cm and 5 to 10 cm) were extracted three times with acetonitrile:acetic acid (70:30). The volume of the combined extracts was measured, then subsamples were radioassayed by LSC. Extracts were diluted with water and partitioned three times with methylene chloride. The aqueous phase and combined methylene chloride phase were counted (LSC). The methylene chloride phase was then taken to dryness (rotary evaporation). Residues in methanol were transferred to vials; after solvent evaporation (N_2) samples were stored frozen until TLC analysis.

Extracted soils were air dried and subsamples radioassayed by LSC.

Column eluates (combined for each radiochemical) were evaporated to dryness (vacuum). Residues in methanol were filtered and transferred to vials; after solvent evaporation (N_2) samples were stored in a freezer until TLC analysis.

Residues from the column eluate or soil extracts were redissolved in methanol prior to TLC on silica gel plates. Four mobile phases were used: either a 75:25:1, 85:15:0.5, or 90:10:0.5 chloroform:methanol:acetic acid or a 65:25:10 ethyl acetate:2-propanol:water system. Radioactive areas were detected by autoradiography. Quantification of the radioactivity was accomplished by zonal scraping followed by LSC.

Results

The post-leaching ^{14}C distributions in each soil and the quantity in leachate are summarized in Table 4. Most of the recovered activity was in the top 10 cm of the soil columns: 76% to 96% for the triazole label and 81% to 85% for the phenyl label. The corresponding amounts recovered in leachate were 1.0% to 6.3% (triazole) and 5.0% to 6.0% (phenyl). Reported ^{14}C recoveries ranged from 93% to 110% of that applied to the columns.

^{14}C Residues in the pre-leached aged soils were largely (>83%) extractable. Approximately 80% of the triazole label recovered from the top 10 cm of the leached columns was extractable; the corresponding figure for the phenyl label was ~60%. Extracted activity from both unleached and leached soils was shown to be largely (86% to 92%) parent, with 6% to 10% present as an unidentified polar metabolite. The unidentified polar metabolite was also reported, but not quantified, in column eluate.

A K_d value of 40 was calculated for RH-3866 from $K_d = \text{pesticide adsorbed } (\mu\text{g/kg}) / \text{pesticide in solution } (\mu\text{g/L})$.

The post-leaching distribution of residues from the 2,4-D treated columns suggests that mobility of the compound was low.

Table 4. Distribution of ^{14}C residues in soil columns and leachate.^a

Depth (cm)	% Recovered ^{14}C					
	Triazole $^{14}\text{C}^{\text{b}}$		Phenyl $^{14}\text{C}^{\text{c}}$		^{14}C 2,4-D	
	1 ^d	2	1	2	1	2
0-5	79	48	57	59	96	97
5-10	17	28	24	26	3.0	2.0
10-15	1.0	2.4	9.0	5.0	0.6	0.5
15-22.5	1.0	6.3	3.0	2.0	0.2	0.25
22.5-30	0.5	3.0	2.0	2.0	--	--
Leachate	1.0	6.3	5.0	6.0	0.2	0.25

^a Columns leached with 55 mls H_2O /day for 46 days.

^b Triazole-labeled [^{14}C]RH-3866.

^c Phenyl-labeled [^{14}C]RH-3866.

^d Two replicates per treatment.

Conclusions

Most of the activity recovered from silt loam soil columns treated with aerobically aged RH-3866, then leached with the equivalent of 20 inches of rain, was present as parent in the top 10 cm of soil. Activity leached below 10 cm was not identified; an unidentified polar metabolite was reported in the column eluate but no further characterization was performed. Thus the results suggest that RH-3866 residues will not be highly mobile in soils of this textural class.

The registrant's calculation of K_d overestimates the true value. The pesticide concentration should be calculated for the solution in equilibrium with soil in the column. Calculation on the basis of the total leachate volume is inconsistent with the stated definition of K_d . The value of 40 for K_d reported in this study is ~6 times that reported in Study 4 from a batch experiment using the same soil.

Additional deficiencies were noted. Leached soil samples were stored for 2 weeks at room temperature prior to analysis. The effect of this storage was not discussed. The agreement between the duplicate columns for the triazole-labeled [^{14}C]RH-3866 treatment was poor.

Evaluation of this study was hampered by apparent inconsistencies in data (for example overall ^{14}C recoveries) within the text of the report, and also in data reported in tables and text.

STUDY 4

Allen, S.S. May, 1984. Adsorptive and desorptive properties of RH-3866 on soils. Rohm and Haas, Philadelphia, PA. Report No. 310-85-05. Acc. No. 072909. Ref. Vol. 15, Sec 21.

Procedure

Five soils, Hagerstown clay loam, Lakeland sand, Lawrenceville silt loam, Pasquotank sandy loam and Cecil clay (characteristics reported in Table 5), were sieved (1.4 mm) and air dried.

conc. range is too low.
Adsorption: Duplicate aliquots of each soil type were treated with phenyl-labeled [^{14}C]RH-3866 (specific activity 10.28 mCi/g, 99% pure, Lot No. 424.01 in 0.01 N CaCl_2) at 0.025, 0.25, 2.5, or 25 ppm. Control samples were treated with 0.01 N CaCl_2 solution only. The mixtures were shaken vigorously at ambient temperature for 24 hours to establish equilibrium. The samples were centrifuged, the supernatant decanted and the volume measured.

Desorption: After the adsorption procedure was complete, each soil at each concentration level, was shaken for 24 hours with 10 ml portions of 0.01 N CaCl_2 , then centrifuged. This process was repeated twice; the soils were then shaken for 66 hours with 0.01 N CaCl_2 , then centrifuged.

Soils were then oven-dried (100°C) for 24 hours.

Methodology

All supernatants obtained during the adsorption and desorption phases were radioassayed (LSC). Residual ^{14}C activity in the soils was determined by combustion followed by LSC.

The amount of [^{14}C]RH-3866 adsorbed by each soil was calculated from the difference in solution concentration before and after equilibration with soil. Values of adsorption per unit weight of soil and equilibrium solution concentrations were fitted graphically to the Freundlich isotherm equation. This procedure was repeated for the desorption data. The intercepts of these plots (Freundlich "K constants") were used as the coefficients of adsorption/desorption per unit weight of soil (K). Coefficients of adsorption per unit organic carbon were calculated from $K_{\text{OC}} = K \times 100/\%$ organic carbon.

Results

The average percent of added RH-3866 adsorbed by the soils ranged from ~31% for the Lakeland sand to 77% for the Pasquotank sandy loam soil. The average percent RH-3866 that was desorbed from the five soils ranged from 47% (Lawrenceville silt loam and Pasquotank sandy loam) to 61% (Hagerstown clay loam).

Table 6 contains adsorption and desorption Freundlich K values on whole soil (K) and on organic carbon (K_{OC}) bases. Adsorption Freundlich K values ranged from 1.46 to 9.77 and were in the order Pasquotank sandy loam > Lawrenceville silt loam > Hagerstown clay loam > Cecil clay > Lakeland sand.

Table 5. Characteristics of the soils used in the adsorption /desorption study.

Soil	Textural class	Sand	Silt	Clay %	OM ^a	OC ^b	pH	CECC ^c (meq/100 g)
Hagerstown	Clay loam	38	34	28	3.42	1.98	6.4	9.4
Lakeland	Sand	98	0	2	0.95	0.55	5.0	1.7
Lawrenceville	Silt loam	16	58	26	2.05	1.19	6.1	11.9
Pasquotank	Sandy loam	70	20	10	2.90	1.68	7.2	12.5
Cecil	Clay	32	14	54	0.44	0.26	4.7	6.9

^a Organic matter.

^b Organic carbon (from % organic matter/1.724).

^c Cation exchange capacity.

Table 6. Adsorption/Desorption Parameters for ^{14}C RH-3866 on five soils.^a

Soil type	Adsorption			Desorption		
	K^b	K_{oc}^c	$1/n^d$	K^b	K_{oc}^c	$1/n^d$
Hagerstown clay loam	4.44	226	0.89	1.19	6.01	0.88
Lakeland sand	1.46	266	0.89	0.47	85.5	0.92
Lawrenceville silt loam	7.08	596	0.88	4.18	351	0.87
Pasquotank sandy loam	9.77	582	0.85	4.08	243	0.78
Cecil clay	2.39	920	0.91	0.58	223	0.97

^a Parameters obtained using the Freundlich equation.

^b Freundlich K value.

^c Coefficient of adsorption per unit organic carbon.

^d Slope of the log-log plot.

Conclusions

This study provides information on the sorption and mobility of the parent compound only. Freundlich K values for adsorption suggest that RH-3866 will be of intermediate mobility in a range of soil types. Since adsorption of RH-3866 by these soils does not appear related to organic carbon content, K values on whole soil, rather than organic carbon bases are more appropriate for interpretation.

The registrant relates variation in sorption of RH-3866 among soils to pH and cation exchange capacity. This analysis is based on correlation coefficients of 0.805 and 0.811 between Freundlich K values and CEC and pH, respectively.

The value of the desorption Freundlich "K constants" presented are doubtful in view of the gross differences between final sorption and initial desorption conditions.

Minor inconsistencies in data reporting were present in this study.

STUDY 5

Allen, S.S. and D.R. Streelman. July, 1983. The octanol/water partition coefficient of RH-3866. Technical Report No. 310-83-18. Rohm and Haas, Philadelphia, PA. Acc. No. 072907. Ref. Vol. 13, Sec. 25.

Procedure

Equal volumes of octanol-saturated water and either 2.19 ppm, 10.3 ppm or 48.4 ppm, 3,5-triazole-labeled [^{14}C]RH-3866 (specific activity 10.98 mCi/g, 99% in watersaturated octanol) solutions were mixed for 15 minutes. The mixtures were centrifuged for 1 hour and the phases separated.

Methodology

Each fraction was radioassayed in triplicate by LSC.

Results

Reported ^{14}C recoveries based on initial RH-3866 solution concentrations ranged from 95.2 to 100.3%.

Recoveries of RH-3866 in the octanol and water fractions and calculated partition coefficients (K_{OW}) are reported in Table 7.

K_{OW} values measured increased with pesticide concentration.

Table 7. Octanol/water partition coefficient (K_{OW}) measured at three RH-3866 concentrations.

Initial concentration (ppm) ^a	Concentration in octanol (ppm)	Concentration in water (ppm)	K_{OW}
2.19	2.140	0.0029	738
2.19	2.079	0.0030	693
10.3	10.08	0.0108	933
10.3	10.33	0.0109	948
48.4	47.81	0.0500	956
48.4	47.93	0.0501	957

^a In water-saturated octanol.

Conclusions

Reported values for the octanol/water partition coefficient of RH-3866 ranged from 693 to 957. The variation in observed values was not discussed.

Schraubelt

EXPERIMENTAL PROGRAM AND APPLICATION INFORMATION

Directions for use

Two formulations of the fungicide RH-3866 are to be evaluated: RH-3866 40 W, a 40% wettable powder formulation and RH-3866 2E, 2 lb ai/A gallon emulsifiable concentrate. Proposed application rates are summarized in Table 8.

Table 8. Uses and application rates of RH-3866.

Formulation	Proposed crop/disease use	Application rate	Maximum application ^a (per acre per crop season)
RH-3866 2E	✓ Wheat/leaf, stem, strip rust	0.5 to 0.75 pints/A	2 pints
	✓ Wheat/powdery mildew	1.0 pints/A	
	✓ Wheat/spot, glume blotch and tan spot	1.0 pint/A	
RH-3866 2E	✓ Turf grass/broad spectrum	0.5 to 1.0 pint/A	2 pints
RH-3866 40W	✓ Wheat/leaf, stem, strip rust	0.3 to 0.16 lb ai/A	1.25 lb
	✓ Wheat/powdery mildew	0.6 lb/A	
	✓ Wheat/spot, glume blotch and tan spot	0.6 lb/A	
RH-3866 40W	✓ Apple/scab	2-8 oz/A	5 lb *
	✓ Apple/powdery mildew	6-12 oz/A	
RH-3866 40W	✓ Grapes/powdery mildew	2-5 oz/A	1 lb
	✓ Grapes/black rot	2-5 oz/A	
RH-3866 40W	✓ Turf grass/broad spectrum	0.3-0.6 lb/A	--b

^a Multiple applications may be necessary for all crops/diseases.

^b Maximum application rate unclear-reported as 1 pint (per acre per crop season).

Experimental program

The planned experimental program is summarized in Table 9. The program is to encompass small scale trials conducted by Experimental Stations, as well as larger scale "grower trials".

Table 9. Summary of proposed experimental program for RH-3866.

Crop	Experiment station trials		Grower trials		
	States ^a	Total ai ^b	States ^a	Acres ^c	Total ai ^b
Wheat	36	144	36	3600	1800
Apples	21	84	21	660	1320
Grapes	11	44	11	560	1120
Turf grass	4	16	4	320	320

^a Number of states involved in proposed program.

^b Total pounds of ai to be used.

^c Number of acres to be treated (reported for grower trials only).

EXECUTIVE SUMMARY

RH-3866 appears stable to hydrolysis at pHs 5, 7, or 9. However, the temperature at which the test solutions were maintained was not reported.

Tentative results (incubation temperature not reported) indicate that RH-3866 is metabolized under aerobic conditions in a silt loam soil to 1,2,4-triazole, CO₂ and a non-extractable form. Initial half-lives were 61 and 71 days respectively for triazole- and phenyl-labeled RH-3866 (calculated from data for up to 62 days of incubation). However, degradation was slower with increased aging; after 240 days up to 37% of recovered ¹⁴C was still present as parent. Tentative results (incubation temperature not reported) indicated that RH-3866 was not appreciably metabolized within 62 days of anaerobic incubation in a silt loam soil.

A batch study indicated that parent RH-3866 was of intermediate mobility in a range of soil types. Aged RH-3866 residues were not extensively leached in a silt loam soil column study.

Estimates of the octanol/water partition coefficient for RH-3866 ranged from 693 to 957.

Recommendations

Available data are insufficient to fully assess the environmental fate of RH-3866. The submission of data relative to EUP requirements (Subdivision N) is summarized below:

Hydrolysis studies: One study (Allen, 1984, Acc. No. 072909) was submitted and reviewed. This study is scientifically valid. However, in order to satisfy Guidelines Requirements the temperatures at which the test solutions were maintained must be reported.

Aerobic soil metabolism: One study (Ackerman, 1984, Acc. No. 072907) was submitted and reviewed. This study may provide useful data for EUP requirements, however, the incubation temperature must be reported. In addition, for full registration, data from a longer sampling period may be required (Guidelines Requirements are for up to 12 months posttreatment).

Anaerobic soil metabolism: One study (Ackerman, 1984, Acc. No. 072907) was submitted, reviewed and found to be scientifically valid. However, the temperature at which samples were incubated must be reported.

Leaching and adsorption/desorption studies: Two studies (Allen, 1984, Acc. No. 072909 and Ackerman, 1984, Acc. No. 072909) were submitted and reviewed. These data are adequate to support the proposed EUP. However, further information on the mobility of soil metabolites is required for full registration.

Confined accumulation studies on rotational crops: No data were submitted; all data are required.

Laboratory studies of a accumulation in fish: No bioaccumulation studies were submitted; all data are required.

References

Ackerman, I.B. June, 1984. Laboratory leaching study with RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-09. Acc. No. 072909.

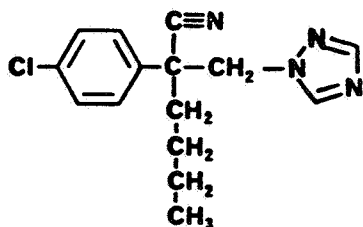
Ackerman, I.B. July, 1984. Laboratory soil metabolism of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-14. Acc. No. 072907.

Allen, S.S. May, 1984. A hydrolysis study of RH-3866. Rohm and Haas, Philadelphia, PA. Report No. 310-84-04. Acc. No. 072909.

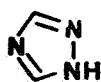
Allen, S.S. May, 1984. Adsorptive and desorptive properties of RH-3866 on soils. Rohm and Haas, Philadelphia, PA. Report No. 310-85-05. Acc. No. 072909.

Allen, S.S. and D.R. Streelman. July, 1983. The octanol/water partition coefficient of RH-3866. Technical Report No. 210-83-18. Rohm and Haas, Philadelphia, PA. Acc. No. 072907.

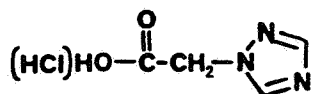
APPENDIX
STRUCTURE OF RH-3866
AND
TLC STANDARDS USED IN STUDY 1



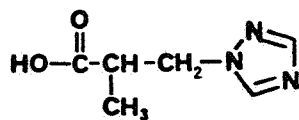
RH-3866 (α -butyl- α -[4-chlorophenyl]-
1-H-1,2,4-triazole-1-propanenitrile)



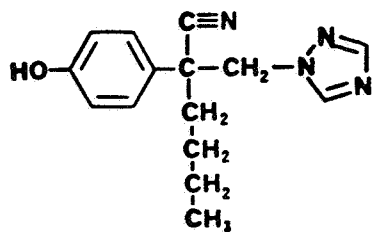
RH-5076 (1,2,4-triazole)



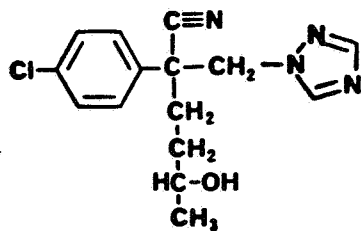
RH-4098



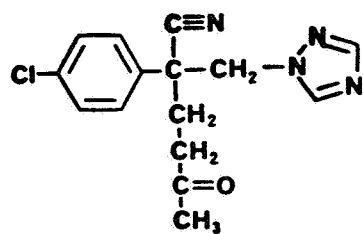
RH-3968



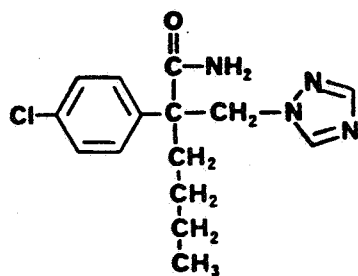
RH-8503



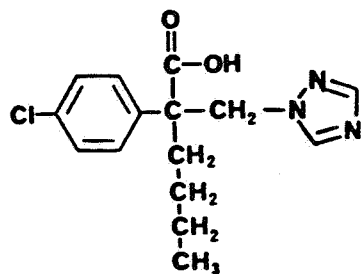
RH-9090



RH-9089



RH-7262



RH-5474